



Raman scattering measures fluid composition in IC engines

Paul Miles and Matt Dilligan of CalTech have recently employed broadband Raman scattering to determine the in-cylinder gas composition in an internal combustion engine. With the advent of high-quality, scientific charge-coupled device detectors and well-corrected imaging spectrographs, it has now become feasible to apply Raman scattering with broadband detection to simultaneously measure all the major species of combustion at multiple points along a laser beam. Such measurements are important for examining the mixing of the fuel and air and of the fresh charge with the burnt residual gases, as well as for understanding the influence of mixture composition on such phenomena as misfire and cyclic variability.

As part of a cooperative research and development agreement with General Motors, the apparatus depicted

in Figure 1 was developed to make these measurements. Light scattered from a 532 nm pulsed laser beam is collected and focused onto the

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entrance slit of an imaging spectrograph, where it forms an image of a length of the original beam. The imaging spectrograph simply disperses the image at the entrance slit spectrally, resulting in multiple images at the detector plane. Each detector plane image corresponds to light scattered from a particular molecular species. By examining the intensity at various positions along these images it is pos-

sible to determine the composition of the in-cylinder gases at the corresponding positions along the laser beam. With broadband collection (over 100 nm in the current system) the major species of combustion – CO_2 , O_2 , N_2 , CO , Fuel, and H_2O – can all be monitored simultaneously.

Mean species mole fractions measured from the beginning of the intake stroke, 0 CAD, to the top of the compression stroke, 360 CAD, are shown in Figure 2. These measurements demonstrate how the burnt residuals (CO_2 and H_2O) are displaced and eventually mix with the fresh charge (O_2 and C_3H_8).

Work is continuing to extend the measurement technique to obtain instantaneous, temporally resolved measurements of the gas composition, and to obtain an absolute measure of the number density of each species.

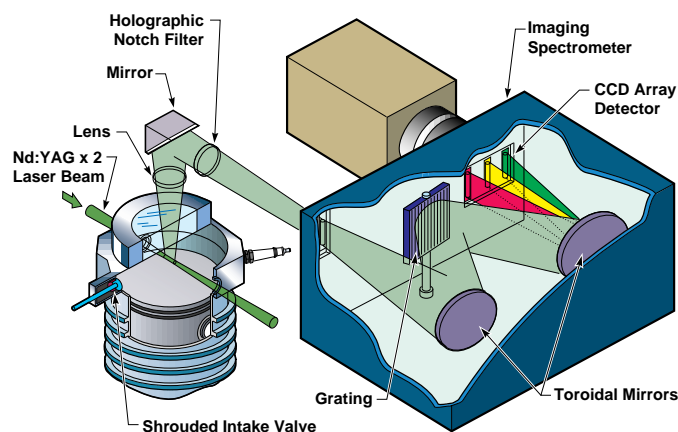


Figure 1. Schematic of the experimental apparatus employed for broadband, multi-point Raman scattering measurements.

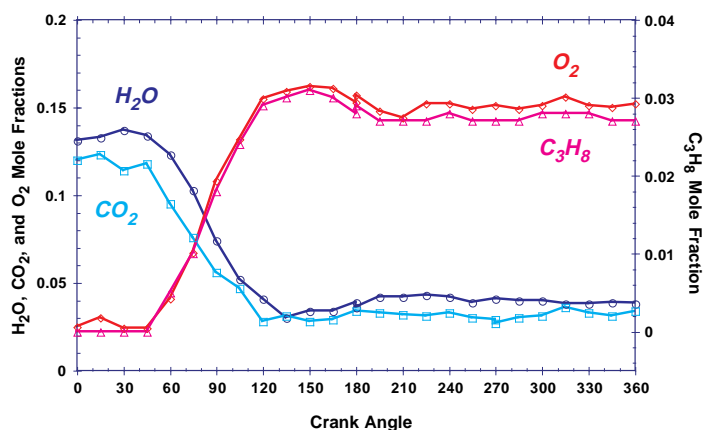


Figure 2. Mean mole fractions of the major species of combustion measured in a firing IC engine.

Biomass pyrolysis conditions affect oil combustion

A team composed of Christopher Shaddix, Sidney Huey, Paul Tennison, and Nancy Yang is investigating the combustion behavior of biomass pyrolysis oils, a potential fuel source for electric power generation. The team works closely with researchers from the National Renewable Energy Laboratory, who produce and analyze the pyrolysis oils. This project is sponsored by the Department of Energy's Office of Utility Technologies, Biomass Power Program.

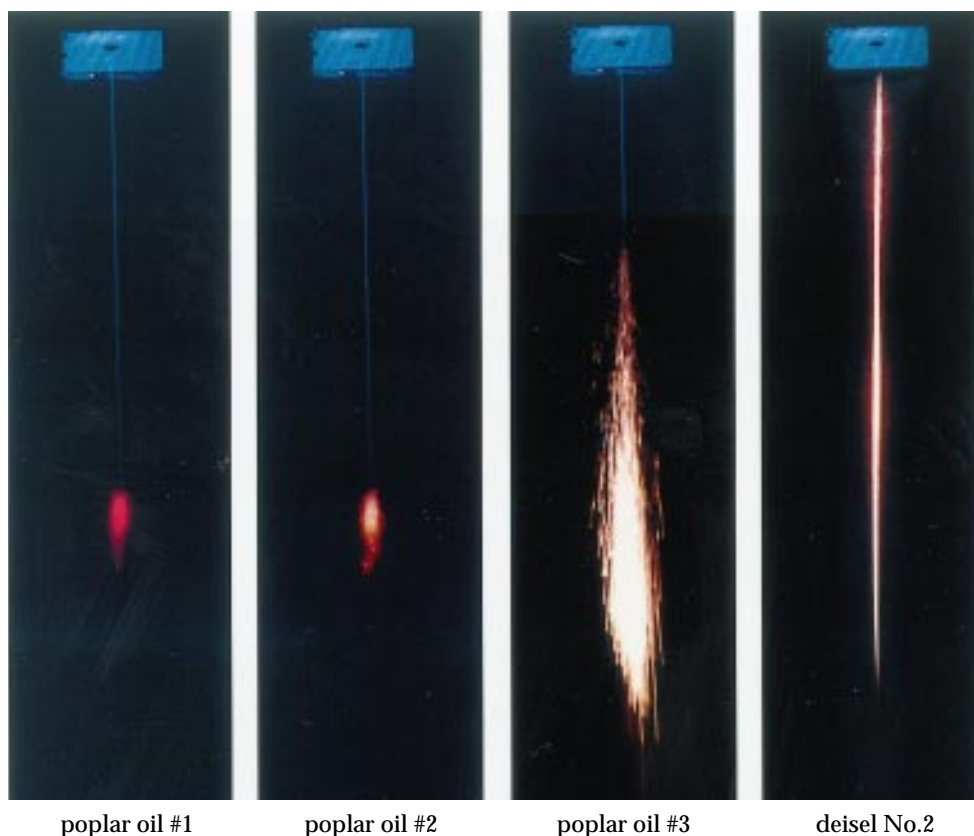
Fast-growing herbaceous or woody biomass sources offer the promise of an indigenous, renewable energy supply with nearly zero net CO₂ production when grown on a sustainable basis. While raw biomass can be burned directly to produce electricity, pyrolysis liquids generated from biomass can have significantly greater economic value due to their projected use in heavy-duty diesel engines or gas turbines. In contrast to conventional fuel oils, biomass oils are characterized by a wide range of molecular weights, high water and oxygen contents, low pH, and high viscosity.

The combustion behavior of three oils produced from the same poplar feedstock was recently evaluated using Sandia's Biomass Fuels Combustion System (BFCS). The BFCS features a quartz-walled laminar-flow combustion reactor with aerodynamic droplet generation, a high-resolution, back-lit stroboscopic video imaging system, and a condensed-phase sampling probe. The three oils differ in the extent of thermal "cracking" experienced by the pyrolysis vapors during their production and thus have different water and oxygen contents.

As shown in the figure, the droplet combustion of the poplar oils differs from that of diesel No. 2 oil, a standard petroleum fuel oil. The biomass oils initially burn quiescently with a faint blue flame before experiencing a violent microexplosion, or sudden formation and release of fuel vapor from interior regions of the droplet. The timing and intensity of this microexplosion event varies significantly among the three poplar oils, with the oil having the highest water content (and lowest oxygen content), poplar

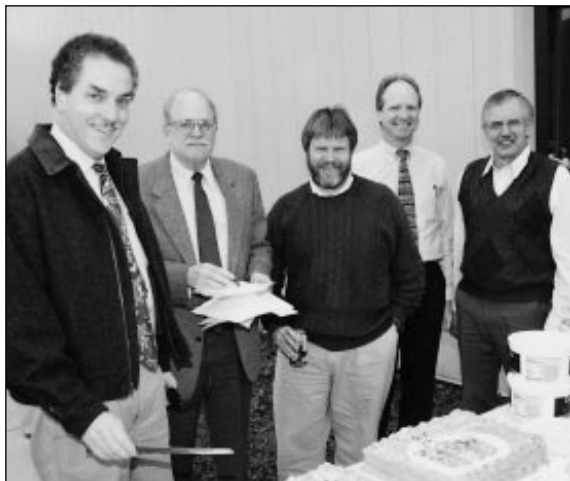
oil #1, experiencing the most complete microexplosion and the oil having the highest oxygen content (and lowest water content), poplar oil #3, microexploding early and relatively ineffectually. This latter oil shows disruptive, sooty burning of the droplets after the initial microexplosion, and some coke particulate production is observed.

As is apparent in the figure, the biomass oils that experience very effective microexplosions have significantly shorter droplet burnout times than the diesel oil, despite having much lower measured burning rates during the quiescent burning stage. The occurrence of these microexplosions in practical combustors could be critical to achieving rapid dispersal of the liquid fuel into the surrounding air, necessary for complete combustion of the oil and low NO_x production. Experiments are being initiated in Sandia's Spray Combustion Facility to evaluate the combustion characteristics of these biomass oils in practical spray flames. 🔥



Time-exposure photographs of droplet combustion in the laminar flow reactor of the CRF Biomass Fuels Combustion System.

CRF celebrates 15th anniversary



The Combustion Research Facility celebrated its 15th anniversary on March 6 with an informal pizza-and-cake lunch on the outdoor patio. Shown here are some of the original staff of the CRF: Bill McLean, Bill (Robby) Robinson, Jim Miller, Mike Dyer, and Don Hardesty. The following day, Sandia/California celebrated its 40th anniversary.



Aram Schiffmann (left) recently completed postdoctoral research with Dave Chandler (center) and is taking a position with Coherent Laser Company. David Neyer (right) is currently working with Dave Chandler readying a new visitor facility at the Combustion Research Facility for the study of chemical dynamics.



Basic Energy Sciences research reviewed

March 13-15 saw the annual peer review of basic research supported at the CRF by the Department of Energy's Office of Basic Energy Sciences, Chemical Sciences Division. This year the review focused on research in reacting flows and diagnostics. Seated left to right are Bill Kirchhoff (DOE) and the reviewers, Dr. Kermit Smyth (National Institute of Standards and Technology), Prof. Paul Ewart (University of Oxford), Dr. Sanjay Correa (General Electric Research Center), and Prof. M. Godfrey Mungal (Stanford University.) Standing are Frank Tully, George Fisk, Allan Laufer (DOE), Bill McLean, Prof. Robert Goulard (George Washington University/DOE), and Larry Rahn.

Kurt Iskra (top right) and Juergen Flieser (bottom left) are Ph.D. students from the Technical University of Graz, Austria. They participated in laser diagnostic development experiments with Roger Farrow (top left) and David Rakestraw (bottom right) for two months. During that time they were able to get first-hand experience with numerous spectroscopic methods including coherent anti-Stokes Raman scattering, degenerate four-wave mixing, laser-induced fluorescence, and cavity ringdown laser absorption spectroscopy. Kurt and Juergen plan to apply many of these techniques in ongoing combustion research at their university in Graz.



New turbulence model developed

Fluid turbulence plays a key role in many energy conversion processes and other engineering and geophysical applications. It is difficult to incorporate the range of turbulence phenomena relevant to these applications in a computationally affordable model. A common approach is to compute explicitly the large-scale flow, or its time average, with small-scale effects subsumed into an effective viscosity. In an effort to overcome limitations of this approach, Alan Kerstein has developed a new turbulence modeling strategy.

In earlier studies of mixing processes in turbulent flows (*CRF News* 17:3), Alan showed that key mechanisms of multidimensional mixing can be captured by a one-dimensional formulation that he termed the 'linear eddy model.' Fully resolved simulations are affordable with this formulation, so fine-scale processes can be treated in a physically sound manner.


This formulation simulates mixing in a specified flow. To predict the flow, Alan has now introduced a one-dimensional velocity profile that evolves according to a random process. The parameters of this process depend on the velocity profile. A self-contained formulation is obtained, involving minimal empiricism.

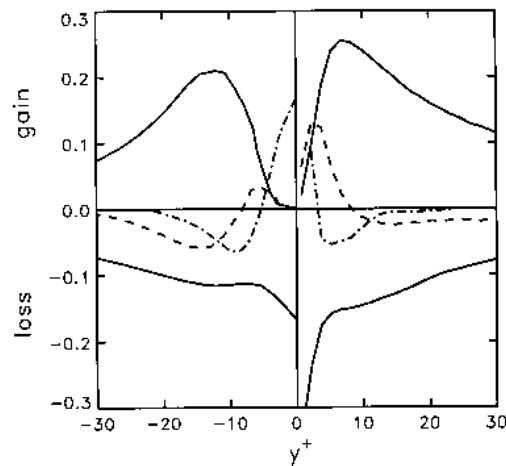
Flows of interest are simulated by applying appropriate initial and boundary conditions to the velocity profile. The fully resolved simulations do not require an effective viscosity assumption, with its attendant limitations.

This modeling strategy, termed 'one-dimensional turbulence,' reproduces many known features of turbulence microstructure (notably, the inertial range turbulent cascade) and macrostructure (notably, similarity scalings governing the decay of homogeneous turbulence and the growth of free shear flows and boundary layers).

This unification of diverse phenomena within a common modeling framework is novel. New predictive capabilities have been demonstrated with regard to fluctuation properties of various flows and mixing processes within these flows.

The figure shows an illustrative example. The structure of turbulent flow near a wall transitions from viscous dominance immediately adjacent to the wall to fully developed turbulence far from the wall. Previous models describe the mean flow and certain second-order fluctuation properties in near-wall flow. The plotted profiles provide the first demonstration that a statistical model involving minimal empiricism can capture salient features of higher order fluctuation properties (third order in this instance). The only empiricism in the model is an adjustable factor that scales the spatial coordinate.

At present, Alan is investigating the applicability of this modeling strategy to buoyant stratified flows. He anticipates applications to geophysical flows, heat transfer problems, and chemically reacting flows. 



Model prediction of the turbulent kinetic energy budget near a wall, compared to published results (Mansour, Kim, and Moin 1988) based on numerical solution of the exact evolution equation (Navier-Stokes equation). The turbulent kinetic energy is the total kinetic energy (time-averaged) minus the kinetic energy of the mean motion. It is generated by imposed shear, transported by various mechanisms, and dissipated by viscosity. Model (right of centerline) and exact (left of centerline) profiles of wall-layer energetics, in normalized units, are plotted versus a normalized spatial coordinate. Terms of the budget: production (upper solid curve), dissipation (lower solid curve), turbulent transport (dashed curve), viscous transport (dot-dashed curve).

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